Topological Aspect of Knotted Vortex Filaments in Excitable Media*

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Scroll waves exist ubiquitously in three-dimensional excitable media. It's rotation center can be regarded as a topological object called vortex filament. In three-dimensional space, the vortex filaments usually form closed loops, and even linked and knotted. In this letter, we give a rigorous topological description of knotted vortex filaments. By using the ϕ-mapping topological current theory, we rewrite the topological current form of the charge density of vortex filaments and use this topological current we reveal that the Hopf invariant of vortex filaments is just the sum of the linking and self-linking numbers of the knotted vortex filaments. We think that the precise expression of the Hopf invariant may imply a new topological constraint on knotted vortex filaments.

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Scroll waves exist ubiquitously in three-dimensional excitable media. They have been directly observed in three-dimensional chemical[1], physical[2, 3], and biological systems[4]. Specific examples include the Belousov-Zhabotinskii reaction[5], the cardiac muscle[6], and the oxidation of CO on platinum[2]. Recently, scroll waves have drawn great interest and have been studied intensively in many ways because it is believed to be the mechanism of some re-entrant cardiac arrhythmias and fibrillation which is the leading cause of death in the industrialized world[7, 8, 9, 10]. The investigation of properties of scroll waves in excitable media provides insights into the possible behaviors of these processes in the cardiac tissue of animals whose heart wall is thick enough for three-dimensional effects to be significant.

On the other hand, the global behavior of a scroll wave is well described by the motion of its approximate rotation center which is a line defect known as a vortex filament and usually defined in terms of a phase singularity. In three-dimensional excitable media, the vortex filaments is commonly a closed ring, and these vortex filaments can form linked and knotted rings which contract to compact, particle-like bundles[11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21]. The existence of the knotted vortex filaments can be regarded as a topological phenomena in excitable media. In most previous works[16, 17, 18, 19, 20, 21], the topological arguments have been applied to help us understand the topological properties of the vortex filaments and some most important topological constraints on behaviors of the vortex filaments have been investigated. These topological rules may have some important applications in practice. In particular, the topological constraint on knotted vortex filaments is believed to relate to topological characteristic numbers of knotted vortex filament family, such as the winding, the self-linking and the linking numbers[19, 20, 21]. So in research into knotted vortex filaments in excitable media, one should play much attention to these knot characteristics. In this letter, we will use the topological viewpoint to study the knotted vortex filaments with the Hopf invariant[23] which can be used to describe the linkages of knot family in mathematics, and reveal the inner relationship between the Hopf invariant and the topological characteristic numbers of the knotted vortex filaments. We think that this inner relationship may imply a new topological constraint on knotted vortex filaments.

We chose to work with a general two-variable reaction-diffusion system which mathematical description in terms of a nonlinear partial differential equation. This equation is written as

$$\partial_t u = f(u,v) + D_u \nabla^2 u, \quad \partial_t v = g(u,v) + D_v \nabla^2 v, \quad (1)$$

where u and v represent the concentrations of the reagents; ∇^2 is the Laplacian operator in three-dimensional space; $f(u,v)$ and $g(u,v)$ are the reaction functions. Following the description in Ref.[16], we define a complex function $Z = \phi^1 + i\phi^2$, where $\phi^1 = u - u^*$ and $\phi^2 = v - v^*$. Here u^* and v^* are the concentrations of the vortex filaments.

As pointed out in Ref.[24] , the sites of the vortex filaments are just the isolated zero lines of the complex function $Z = \phi^1 + i\phi^2$ in three-dimensional space. By using the topological viewpoints, Zhang et al.[16] derived a topological expression of the charge density of these zero lines, i.e., the vortex filaments, which is written as

$$\vec{\rho}(\vec{x},t) = \sum_{l=1}^{N} W_l \int_{L_l} d\vec{x}\,\delta^3(\vec{x} - \vec{x}_l), \quad (2)$$

where W_l is the topological charge of the l-th vortex filament L_l.This expression reveals the topological structures of vortex filaments. In our topological theory of knotted vortex filaments, the topological structure of the vortex filaments will play an essential role. In order to study the knotted vortex filaments more conveniently, we firstly rewrites the charge density of vortex filaments as a topological current. Now we begin to derive the topological current form of the charge density of vortex filaments. We know that the complex function $Z = \phi^1 + i\phi^2$

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can be regarded as the complex representation of a two-dimensional vector field $\vec{Z} = (\phi^1, \phi^2)$. Let us define the unit vector: $n^a = \frac{\phi^a}{\|\phi\|}(a = 1, 2; \|\phi\|^2 = \phi^a\phi^a = Z^*Z)$. It is easy to see that the zeros of Z are just the singularities of $\vec{n}$. Using this unit vector $\vec{n}$, we define a topological current

$$j^i = \frac{1}{2\pi}\epsilon^{ijk}\epsilon_{ab}\partial_j n^a \partial_k n^b, \quad i, j, k = 1, 2, 3. \tag{3}$$

Apply the ϕ-mapping theory[22, 25, 26], one can obtain

$$j^i = \delta(\vec{\phi})D^i(\frac{\phi}{x}), \tag{4}$$

where $D^i(\frac{\phi}{x}) = \frac{1}{2}\epsilon^{ijk}\epsilon_{ab}\partial_j\phi^a\partial_k\phi^b$ is the Jacobian vector. This delta function expression of the topological current j^i tells us it doesn't vanish only when the vortex filaments exist, i.e., $Z = 0$. The sites of the vortex filaments determine the nonzero solutions of j^i. The implicit function theory shows that under the regular condition[27]

$$D^i(\frac{\phi}{x}) \neq 0, \tag{5}$$

the general solutions of

$$\phi^1(\vec{x}, t) = 0, \quad \phi^2(\vec{x}, t) = 0 \tag{6}$$

can be expressed as

$$x^1 = x_l^1(t, s), \quad x^2 = x_l^2(t, s), \quad x^3 = x_l^3(t, s), \quad l = 1, 2, \cdot, N, \tag{7}$$

which represent the world surface of N moving isolated vortex filaments $L_l(l = 1, 2, \cdots, N)$ with string parameter s. In delta function theory[28], one can prove that in three-dimensional space,

$$\delta(\vec{\phi}) = \sum_{l=1}^{N}\beta_k\int_{L_l}\frac{\delta^3(\vec{x} - \vec{x}_l(s))}{|D(\frac{\phi}{u})|_{\Sigma_l}}ds, \tag{8}$$

where $D(\frac{\phi}{u}) = \frac{1}{2}\epsilon^{jk}\epsilon_{mn}\frac{\partial\phi^m}{\partial u^j}\frac{\partial\phi^n}{\partial u^k}$ and Σ_l is the l-th planar element transverse to L_l with local coordinates (u^1, u^2). The positive integer β_l is the Hopf index of ϕ-mapping, which means that when $\vec{x}$ covers the neighborhood of the zero point $\vec{x}_l(s, t)$ once, the vector field $\vec{\phi}$ covers the corresponding region in ϕ space for β_l times. Meanwhile the direction vector of L_l is given by[25, 26]

$$\frac{dx^i}{ds}|_{\vec{x}_l} = \frac{D^i(\phi/x)}{D(\phi/u)}|_{\vec{x}_l}. \tag{9}$$

Then considering Eqs.(8) and Eqs.(9), we obtain the inner structure of j^i,

$$\begin{aligned} j^i &= \delta(\vec{\phi})D^i(\frac{\phi}{x}) \\ &= \sum_{l=1}^{N}\beta_l\eta_l\int_{L_l}dx^i\delta^3(\vec{x} - \vec{x}_l), \end{aligned} \tag{10}$$

where $\eta_l = sgnD(\frac{\phi}{u}) = \pm 1$ is the Brouwer degree of ϕ-mapping, with $\eta_l = 1$ corresponding to the vortex filament and $\eta_l = -1$ corresponding to the antivortex filament. Compare Eqs.(2) and Eqs.(10) we see that the topological current $\vec{j}$ is just the charge density vector $\vec{\rho}$ of the vortex filament in Ref.[16]. In our theory, the topological charge of the vortex filament L_l is

$$Q_l = \int_{\Sigma_l}\vec{j}\cdot d\vec{\sigma} = W_l = \beta_l\eta_l, \tag{11}$$

in which W_l is just the winding number of $\vec{Z}$ around L_l, the above expression reveals distinctly that the topological charge of vortex filament is not only the winding number, but also expressed by the Hopf indices and Brouwer degrees. The topological inner structure showed in Eq.(11) is more essential than in Eq.(2), this is just the advantage of our topological description of the vortex filaments.

Now let us begin to discuss the topological properties of knotted vortex filaments in excitable media. It is well know that the Hopf invariant is an important topological invariant to describe the topological characteristics of the knot family. In our topological theory of knotted vortex filaments, the Hopf invariant relates to the topological characteristics numbers of the knotted vortex filaments family. In a closed three-manifold M the Hopf invariant is defined as[22, 23]

$$H = \frac{1}{2\pi}\int_M A_i j^i d^3x, \tag{12}$$

in which A_i is a "induced Abelian gauge potential" constructed with the complex function Z. The relationship between the Abelian gauge field strength $F_{ij} = \partial_i A_j - \partial_j A_i$ and the topological current j^i is[26]

$$j^i = \frac{1}{4\pi}\epsilon^{ijk}F_{jk} = \frac{1}{2\pi}\epsilon^{ijk}\epsilon_{ab}\partial_j n^a\partial_k n^b. \tag{13}$$

Substituting Eq.(10) into Eq.(12), one can obtain

$$H = \frac{1}{2\pi}\sum_{l=1}^{N}W_l\int_{L_l}A_i dx^i. \tag{14}$$

It can be seen that when these N vortex filaments are N closed curves, i.e., a family of N knots $\xi_l(l = 1, 2, \cdots, N)$, Eq.(14) leads to

$$H = \frac{1}{2\pi}\sum_{l=1}^{N}W_l\oint_{\xi_l}A_i dx^i. \tag{15}$$

This is a very important expression. Consider a transformation of complex function $Z' = e^{i\theta}Z$, this gives the U(1) gauge transformation of $A_i : A_i' = A_i + \partial_i\theta$, where $\theta \in R$ is a phase factor denoting the U(1) gauge transformation. It is seen that the $\partial_i\theta$ term in Eq.(15) contributes nothing to the integral H when the vortex filaments are closed, hence the expression (15) is invariant

under the U(1) gauge transformation. As pointed out in Ref.[16] , a singular vortex filament is either closed ring or infinite curve, therefore we conclude that the Hopf invariant is a spontaneous topological invariant for the vortex filaments in excitable media.

It is well known that many important topological numbers are related to a knot family such as the self-linking number and Gauss linking number. In order to discuss these topological numbers of knotted vortex filaments, we define Gauss mapping:

$$\vec{m} : S^1 \times S^1 \to S^2, \tag{16}$$

where $\vec{m}$ is a unit vector

$$\vec{m}(\vec{x},\vec{y}) = \frac{\vec{y}-\vec{x}}{|\vec{y}-\vec{x}|}, \tag{17}$$

where $\vec{x}$ and $\vec{y}$ are two points, respectively, on the knots ξ_k and ξ_l (in particular, when $\vec{x}$ and $\vec{y}$ are the same point on the same knot ξ , $\vec{n}$ is just the unit tangent vector $\vec{T}$ of ξ at $\vec{x}$). Therefore, when $\vec{x}$ and $\vec{y}$, respectively, cover the closed curves ξ_k and ξ_l once, $\vec{n}$ becomes the section of sphere bundle S^2. So, on this S^2 we can define the two-dimensional unit vector $\vec{e} = \vec{e}(\vec{x},\vec{y})$. $\vec{e}$, $\vec{m}$ are normal to each other, i.e. ,

$$\begin{aligned} &\vec{e}_1 \cdot \vec{e}_2 = \vec{e}_1 \cdot \vec{m} = \vec{e}_2 \cdot \vec{m} = 0, \\ &\vec{e}_1 \cdot \vec{e}_1 = \vec{e}_2 \cdot \vec{e}_2 = \vec{m} \cdot \vec{m} = 1. \end{aligned} \tag{18}$$

In fact, the gauge field $\vec{A}$ can be decomposed in terms of this two-dimensional unit vector $\vec{e}$: $A_i = \epsilon_{ab} e^a \partial_i e^b - \partial_i \theta$, where θ is a phase factor[25, 26]. Because the $(\partial_i \theta)$ term does not contribute to the integral H, A_i can in fact be expressed as

$$A_i = \epsilon_{ab} e^a \partial_i e^b. \tag{19}$$

Substituting it into Eq.(14), one can obtain

$$H = \frac{1}{2\pi} \sum_{k=1}^{N} W_k \oint_{\xi_k} \epsilon_{ab} e^a(\vec{x},\vec{y}) \partial_i e^b(\vec{x},\vec{y}) dx^i. \tag{20}$$

Noticing the symmetry between the points $\vec{x}$ and $\vec{y}$ in Eq.(17), Eq.(20) should be reexpressed as

$$H = \frac{1}{2\pi} \sum_{k,l=1}^{N} W_k W_l \oint_{\xi_k} \oint_{\xi_l} \epsilon_{ab} \partial_i e^a \partial_j e^b dx^i \wedge dy^j. \tag{21}$$

In this expression there are three cases: (1) ξ_k and ξ_l are two different vortex filaments ($\xi_k \neq \xi_l$), and $\vec{x}$ and $\vec{y}$ are therefore two different points ($\vec{x} \neq \vec{y}$); (2) ξ_k and ξ_l are the same vortex filaments ($\xi_k = \xi_l$), but $\vec{x}$ and $\vec{y}$ are two different points ($\vec{x} \neq \vec{y}$); (3) ξ_k and ξ_l are the same vortex filaments ($\xi_k = \xi_l$), and $\vec{x}$ and $\vec{y}$ are the same points ($\vec{x} = \vec{y}$). Thus, Eq.(21) can be written as three terms:

$$\begin{aligned} H = &\sum_{k=1(k=l,\vec{x}\neq\vec{y})}^{N} \frac{1}{2\pi} W_k^2 \oint_{\xi_k} \oint_{\xi_k} \epsilon_{ab} \partial_i e^a \partial_j e^b dx^i \wedge dy^j \\ &+ \frac{1}{2\pi} \sum_{k=1}^{N} W_k^2 \oint_{\xi_k} \epsilon_{ab} e^a \partial_i e^b dx^i \\ &+ \sum_{k,l=1(k\neq l)}^{N} \frac{1}{2\pi} W_k W_l \oint_{\xi_k} \oint_{\xi_l} \epsilon_{ab} \partial_i e^a \partial_j e^b dx^i \wedge dy^j . \end{aligned} \tag{22}$$

By making use of the relation $\epsilon_{ab} \partial_i e^a \partial_j e^b = \frac{1}{2} \vec{m} \cdot (\partial_i \vec{m} \times \partial_j \vec{m})$, the Eq.(22) is just

$$\begin{aligned} H \ = \ &\sum_{k=1(\vec{x}\neq\vec{y})}^{N} \frac{1}{4\pi} W_k^2 \oint_{\xi_k} \oint_{\xi_k} \vec{m}^*(dS) \\ &+ \frac{1}{2\pi} \sum_{k=1}^{N} W_k^2 \oint_{\xi_k} \epsilon_{ab} e^a \partial_i e^b dx^i \\ &+ \sum_{k,l=1(k\neq l)}^{N} \frac{1}{4\pi} W_k W_l \oint_{\xi_k} \oint_{\xi_l} \vec{m}^*(dS), \end{aligned} \tag{23}$$

where $\vec{m}^*(dS) = \vec{m} \cdot (\partial_i \vec{m} \times \partial_j \vec{m}) dx^i \wedge dy^j \, (\vec{x} \neq \vec{y})$ denotes the pullback of the S^2 surface element.

In the following we will investigate the three terms in the Eq.(23) in detail. Firstly, the first term of Eq.(23) is just related to the writhing number $Wr(\xi_k)$ of ξ_k[29, 30]

$$Wr(\xi_k) = \frac{1}{4\pi} \oint_{\xi_k} \oint_{\xi_l} \vec{m}^*(dS). \tag{24}$$

For the second term, one can prove that it is related to the twisting number $Tw(\xi_k)$ of ξ_k

$$\begin{aligned} \frac{1}{2\pi} \oint_{\xi_k} \epsilon_{ab} e^a \partial_i e^b dx^i \quad &= \frac{1}{2\pi} \oint_{\xi_k} (\vec{T} \times \vec{V}) \cdot d\vec{V} \\ &= Tw(\xi_k), \end{aligned} \tag{25}$$

where $\vec{T}$ is the unit tangent vector of knot ξ_k at $\vec{x}$ ($\vec{m} = \vec{T}$ when $\vec{x} = \vec{y}$) and $\vec{V}$ is defined as $e^a = \epsilon^{ab} V^b (\vec{V} \perp \vec{T}, \vec{e} = \vec{T} \times \vec{V})$. In terms of the White formula[29, 30]

$$SL(\xi_k) = Wr(\xi_k) + Tw(\xi_k), \tag{26}$$

we see that the first and the second terms of Eq.(23) just compose the self-linking numbers of knots.

Secondly, for the third term, one can prove that

$$\begin{aligned} &\frac{1}{4\pi} \oint_{\xi_k} \oint_{\xi_l} \vec{m}^*(dS) \\ &= \frac{1}{4\pi} \epsilon^{ijk} \oint_{\xi_k} dx^i \oint_{\xi_l} dy^j \frac{(x^k - y^k)}{\|\vec{x} - \vec{y}\|^3} \\ &= Lk(\xi_k, \xi_l) \quad (k \neq l), \end{aligned} \tag{27}$$

where $Lk(\xi_k, \xi_l)$ is the Gauss linking number between ξ_k and ξ_l[31]. Therefore, from Eqs.(24), (25), (26) and (27), we obtain the important result:

$$H = \sum_{k=1}^{N} W_k^2 SL(\xi_k) + \sum_{k,l=1(k\neq l)}^{N} W_k W_l Lk(\xi_k, \xi_l). \quad (28)$$

This precise expression just reveals the relationship between H and the self-linking and the linking numbers of the vortex filaments knots family. Since the self-linking and the linking numbers are both the invariant characteristic numbers of the vortex filaments knots family in topology, H is an important topological invariant required to describe the linked vortex filaments in excitable media.

So far, we obtained a more essential topological formulary of charge density of knotted vortex filaments and revealed the topological inner relationship of between the Hopf invariant and the self-linking and the linking numbers of knotted vortex filaments. We conclude that the Hopf invariant is just the sum of the linking and self-linking numbers of the knotted vortex filaments. In the present study, it should be pointed out that, when we discussed the topological properties of the vortex filaments, the regular condition $D^i(\frac{\phi}{x}) \neq 0$ must be satisfied. Now the question is coming, when this condition fails, what will happen about the vortex filaments? The answer is related to the evolution of the vortex filaments[25, 26]. As we all known that the evolution of the vortex filaments which include generating, annihilating, splitting, or merging may obey some topological constraints. These constraints usually relate to the topological numbers of the vortex filaments, such as the topological charges and linking numbers. So it is naturally to think that the precise expression Eq.(28) of Hopf invariant may imply a new topological constraint on the behavior of the knotted vortex filaments. What the rigorous description of this possible new constraint is will be investigated in our further works.

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